Self-Consistent Vertex Correction Analysis for Iron-Based Superconductors: Mechanism of Coulomb-Interaction-Driven Orbital Fluctuations

Seiichiro ONARI[1] and Hiroshi KONTANI[2]
[1] *Department of Applied Physics, Nagoya University and JST, TRIP, Furo-cho, Nagoya 464-8602, Japan.*
[2] *Department of Physics, Nagoya University and JST, TRIP, Furo-cho, Nagoya 464-8602, Japan.*

(Dated: February 26, 2013)

We study the mechanism of orbital/spin fluctuations due to multiorbital Coulomb interaction in iron-based superconductors, going beyond the random-phase-approximation. For this purpose, we develop a self-consistent vertex correction (SC-VC) method, and find that multiple orbital fluctuations in addition to spin fluctuations are mutually emphasized by the "multimode interference effect" described by the VC. Then, both the antiferro-orbital and ferro-orbital (=nematic) fluctuations simultaneously develop for $J/U \sim 0.1$, both of which contribute to the s-wave superconductivity. Especially, the ferro-orbital fluctuations give the orthorhombic structure transition as well as the softening of shear modulus C_{66}.

PACS numbers: 74.70.Xa, 74.20.-z, 74.20.Rp

Since the discovery of iron-based superconductors, the mechanism of high-$T_{\rm c}$ superconductivity has been studied very actively. Theoretically, both the spin-fluctuation-mediated $s_\pm$-wave state (with sign reversal of the gap between hole-pocket (h-pocket) and electron-pocket (e-pocket)) [1–5] and the orbital-fluctuation-mediated s_{++}-wave state (without sign reversal) [6, 7] had been proposed. The latter scenario is supported by the robustness of $T_{\rm c}$ against impurities in many iron-pnictides [8–12]. Possibility of impurity-induced crossover from $s_\pm$ to s_{++} states had been discussed theoretically [3, 6]. Also, orbital-independent gap observed in $BaFe_2(As,P)_2$ and $(K,Ba)Fe_2As_2$ by laser ARPES measurement [13, 14] as well as the "resonance-like" hump structure in the neutron inelastic scattering [15] are consistent with the orbital fluctuation scenario.

Nature of orbital fluctuations has been studied intensively after the discovery of large softening of the shear modulus C_{66} [16–18] and renormalization of phonon velocity [19] observed well above the orthorhombic structure transition temperature T_S. Consistently, a sizable orbital polarization is observed in the orthorhombic phase [20, 21]. Moreover, the "electronic nematic state" with large in-plane anisotropy of resistivity or magnetization well above T_S and $T_{\rm c}$ [22, 23], also indicates the occurrence of (impurity-induced local) orbital order [24].

Origin of orbital order/fluctuation had been actively discussed, mainly based on the multiorbital Hubbard model with intra (inter) orbital interaction U (U') and the exchange interaction $J = (U - U')/2 > 0$ [6, 25]. We had focused attention to a good *inter-orbital nesting* of the Fermi surfaces shown in Fig. 1 (a): Although moderate orbital fluctuations are induced by U' in the random-phase-approximation (RPA), the spin susceptibility due to the intra-orbital nesting, $\chi^s(\boldsymbol{q})$, is the most divergent for $J > 0$ (*i.e.*, $U > U'$). Since $J/U \approx 0.12-0.15$ according to the first-principle study [26], the RPA fails to explain experimental "nonmagnetic" structure transition. This situation is unchanged even if the self-energy correction is considered in the fluctuation-exchange (FLEX) approximation [27].

To explain the strong development of orbital fluctuations, we had introduced a quadrupole interaction [6]:

$$H_{\rm quad} = -g \sum_i \left(\hat{O}^i_{xz}\hat{O}^i_{xz} + \hat{O}^i_{yz}\hat{O}^i_{yz} \right) \tag{1}$$

where g is the coupling constant, and $\hat{O}_\gamma$ is the charge quadrupole operator ;$\gamma = xz, yz, xy, x^2-y^2, 3z^2-r^2$. (Hereafter, x, y-axes (X, Y-axes) are along the nearest Fe-Fe (Fe-As) direction.) This term is actually caused by the electron-phonon (e-ph) coupling due to in-plane Fe-ion oscillations [6, 14, 27]. Since $\hat{O}_{xz(yz)}$ induces the inter-orbital scattering, strong antiferro (AF) orbital fluctuations develop for $g \gtrsim 0.2$eV owing to a good inter-orbital nesting. We also studied the vertex correction (VC) beyond the RPA [28], and obtained strong enhancement of ferro-quadrupole ($\hat{O}_{x^2-y^2} \propto \hat{n}_{xz} - \hat{n}_{yz}$) susceptibility $\chi^c_{x^2-y^2}(\mathbf{0})$, which causes the orthorhombic structure transition and the softening of C_{66} [28]. This "nematic fluctuation" is derived from the interference of two AF orbitons due to the symmetry relation $\hat{O}_{x^2-y^2}(\mathbf{0}) \sim \hat{O}_{XZ}(\boldsymbol{Q}) \times \hat{O}_{YZ}(-\boldsymbol{Q})$, where $\hat{O}_{XZ(YZ)} = [\hat{O}_{xz} + (-)\hat{O}_{yz}]/\sqrt{2}$. Then, it was natural to expect that such multi-orbiton interference effect, which is given by the VC while dropped in the RPA, induces large "Coulomb-interaction-driven" orbital fluctuations.

In this letter, we study the orbital and spin fluctuations in iron-based superconductors by considering the multiorbital Coulomb interaction with $U = U' + 2J$ and $J/U \sim O(0.1)$. We develop the self-consistent-VC (SC-VC) method, and find that both ferro-$O_{x^2-y^2}$ and AF-$O_{xz/yz}$ fluctuations strongly develop even for $J/U \sim 0.1$, due to the inter-orbital nesting and the positive interference between multi-fluctuation (orbiton+magnon) modes. This result leads to a conclusion that RPA *underestimates* the orbital fluctuations in multiorbital sys-

tems. The present study offers a unified explanation for both the superconductivity and structure transition in many compounds.

Here, we study the five-orbital Hubbard model introduced in Ref. [1]. We denote d-orbitals $m = 3z^2-r^2$, xz, yz, xy, and x^2-y^2 as 1, 2, 3, 4 and 5, respectively. The Fermi surfaces are mainly composed of orbitals 2, 3 and 4 [28]. Then, the susceptibility for the charge (spin) channel is given by the following 25×25 matrix form in the orbital basis:

$$\hat{\chi}^{c(s)}(q) = \hat{\chi}^{\mathrm{irr},c(s)}(q)(1-\hat{\Gamma}^{c(s)}\hat{\chi}^{\mathrm{irr},c(s)}(q))^{-1}, \qquad (2)$$

where $q = (\boldsymbol{q}, \omega_l = 2\pi lT)$, and $\hat{\Gamma}^{c(s)}$ represents the Coulomb interaction for the charge (spin) channel composed of U, U' and J given in Refs. [6, 14]. The irreducible susceptibility in Eq. (2) is given as

$$\hat{\chi}^{\mathrm{irr},c(s)}(q) = \hat{\chi}^0(q) + \hat{X}^{c(s)}(q), \qquad (3)$$

where $\chi^0_{ll',mm'}(q) = -T\sum_p G_{lm}(p+q)G_{m'l'}(p)$ is the bare bubble, and the second term is the VC (or orbiton or magnon self-energy) that is neglected in both RPA and FLEX approximation. In the present discussion, it is convenient to consider the quadrupole susceptibilities:

$$\begin{aligned}\chi^c_{\gamma,\gamma'}(q) &\equiv \sum_{ll',mm'} O_\gamma^{l,l'}\chi^c_{ll',mm'}(q)O_{\gamma'}^{m',m} \\ &= \mathrm{Tr}\{\hat{O}_\gamma\hat{\chi}^c(q)\hat{O}_{\gamma'}\}. \end{aligned}\qquad (4)$$

Non-zero matrix elements of the quadrupole operators for the orbital $2\sim 4$ are $O^{3,4}_{xz} = O^{2,4}_{yz} = O^{2,2}_{x^2-y^2} = -O^{3,3}_{x^2-y^2} = 1$ [28]. Because of the symmetry, the off-diagonal susceptibilities ($\gamma\neq\gamma'$) are zero or very small for $\boldsymbol{q}=\boldsymbol{0}$ and the nesting vector $\boldsymbol{Q}\approx(\pi,0)$ or $\boldsymbol{Q'}\approx(0,\pi)$ [28]. We do not discuss the angular momentum (dipole) susceptibility, $\chi^c_\mu(\boldsymbol{q})\sim\langle\hat{l}_\mu(\boldsymbol{q})\hat{l}_\mu(-\boldsymbol{q})\rangle$, since it is found to be suppressed by the VC. Note that $\hat{O}_{\mu\nu}\propto\hat{l}_\mu\hat{l}_\nu+\hat{l}_\nu\hat{l}_\mu$.

To measure the distance from the criticality, we introduce the charge (spin) Stoner factor $\alpha^{c(s)}_{\boldsymbol{q}}$, which is the largest eigenvalue of $\hat{\Gamma}^{c(s)}\hat{\chi}^{\mathrm{irr},c(s)}(\boldsymbol{q})$ at $\omega_l = 0$: The charge (spin) susceptibility diverges when $\alpha^{c(s)}_{\max}\equiv\max_{\boldsymbol{q}}\{\alpha^{c(s)}_{\boldsymbol{q}}\} = 1$. In a special case $J=0$, the relation $\alpha^s_{\max}=\alpha^c_{\max}$ holds at the momentum $\boldsymbol{Q}$ in the RPA; see Fig. 1 (b). That is, both spin and orbital susceptibilities are equally enhanced at $J=0$, which is unchanged by the self-energy correction in the FLEX approximation [27]. For $J>0$, the spin fluctuations are always dominant ($\alpha^s_{\max}>\alpha^c_{\max}$) in the RPA or FLEX. However, because of large $\hat{X}^c(q)$, the opposite relation $\alpha^s_{\max}\lesssim\alpha^c_{\max}$ can be realized even for $J/U\lesssim 0.1$ in the SC-VC method.

First, we perform the RPA calculation for $n=6.1$ and $T=0.05$, using 32×32 $\boldsymbol{k}$-meshes: The unit of energy is eV hereafter. Figure 1 (c) shows the diagonal quadrupole susceptibilities for $J/U = 0.088$; $\chi^c_\gamma(q)\equiv\chi^c_{\gamma\gamma}(q)$. (The spin susceptibility is shown in Ref. [1].) The Stoner

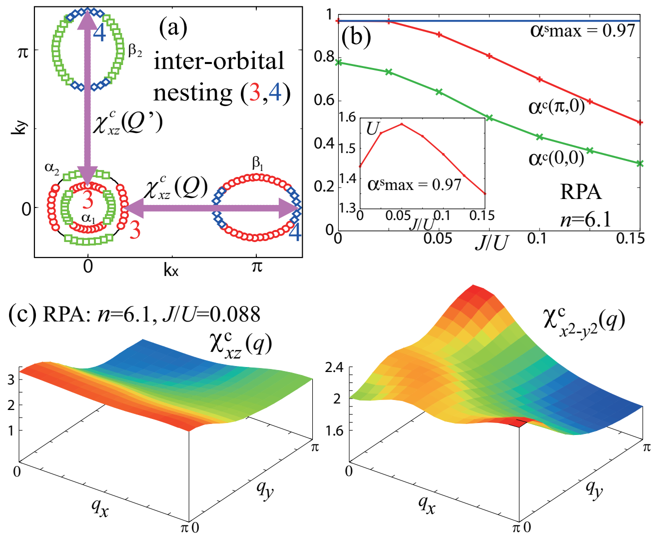

FIG. 1: (color online) (a) Fermi surfaces of iron pnictides. The colors correspond to $2 = xz$ (green), $3 = yz$ (red), and $4 = xy$ (blue), respectively. (b) $\alpha^c_{\boldsymbol{Q}}$, $\alpha^c_{\boldsymbol{0}}$ and U as function of J/U in RPA under the condition $\alpha^s_{\max}=0.97$. (c) $\chi^c_{xz}(\boldsymbol{q})$ and $\chi^c_{x^2-y^2}(\boldsymbol{q})$ given by the RPA for $(J/U,U) = (0.088, 1.53)$.

factors are $\alpha^s_{\max} = 0.97$, $\alpha^c_{\boldsymbol{Q}} = 0.76$, and $\alpha^c_{\boldsymbol{0}} = 0.47$; see Fig. 1 (b). In the RPA, $\chi^c_{xz}(\boldsymbol{Q})$ [$\chi^c_{yz}(\boldsymbol{Q'})$] is weakly enlarged by the inter-orbital $(3,4)$ [$(2,4)$] nesting, while $\chi^c_{x^2-y^2}(\boldsymbol{q})$ is relatively small and AF-like. Thus, the RPA cannot explain the structure transition that requires the divergence of $\chi^c_{x^2-y^2}(\boldsymbol{0})$.

Next, we study the role of VC due to the Maki-Thompson (MT) and Aslamazov-Larkin (AL) terms in Fig. 2 (a), which become important near the critical point [29, 30]. Here, $\hat{X}^{c(s)}(q)\equiv\hat{X}^{\uparrow,\uparrow}(q)+(-)\hat{X}^{\uparrow,\downarrow}(q)$, and wavy lines represent $\chi^{s,c}$. The AL term (AL1+AL2) for the charge sector, $X^{\mathrm{AL},c}_{ll',mm'}(q)$, is given as

$$\begin{aligned}&\frac{T}{2}\sum_k\sum_{a\sim h}\Lambda_{ll',ab,ef}(q;k)\{V^c_{ab,cd}(k+q)V^c_{ef,gh}(-k) \\ &+3V^s_{ab,cd}(k+q)V^s_{ef,gh}(-k)\}\Lambda'_{mm',cd,gh}(q;k),\end{aligned}\qquad (5)$$

where $\hat{V}^{s,c}(q)\equiv\hat{\Gamma}^{s,c}+\hat{\Gamma}^{s,c}\hat{\chi}^{s,c}(q)\hat{\Gamma}^{s,c}$, $\hat{\Lambda}(q;k)$ is the three-point vertex made of three Green functions in Fig. 2 (a) [28], and $\Lambda'_{mm',cd,gh}(q;k)\equiv\Lambda_{ch,mg,dm'}(q;k)+\Lambda_{gd,mc,hm'}(q;-k-q)$. We include all U^2-terms, which are important for reliable results. The expressions of other VCs will be published in future.

Both MT and AL terms correspond to the first-order mode-coupling corrections to the RPA susceptibility: The intra- (inter-) bubble correction gives the MT (AL) term [29]. In single-orbital models, the VC due to MT+AL terms had been studied by the self-consistent-renormalization (SCR) theory [29] or FLEX approximation with VC [30], and successful results had been obtained. In the former (latter) theory, the susceptibility is calculated in the self-consistent (self-inconsistent) way.

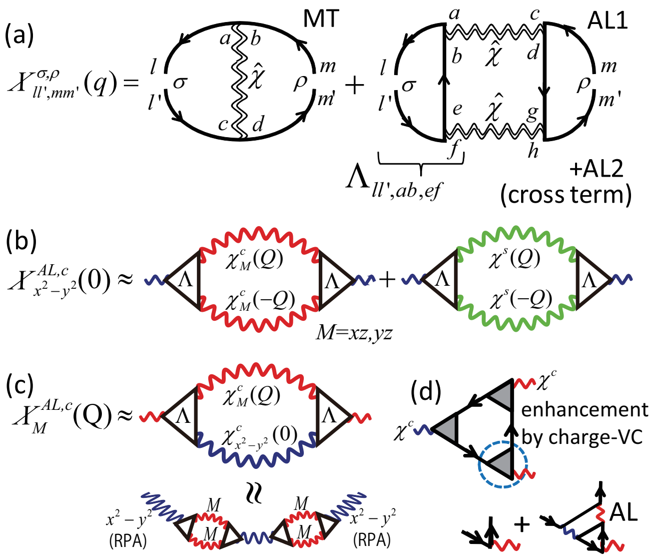

FIG. 2: (color online) (a) The MT and AL terms: The wavy and solid lines are susceptibilities and electron Green functions, respectively. $\Lambda_{ll',ab,ef}$ is the three-point vertex. (b) Dominant AL terms for $\chi^c_{x^2-y^2}(\mathbf{0})$; the first (second) term represents the two-orbiton (two-magnon) process. (c) Dominant AL terms for $\chi^c_M(\boldsymbol{Q})$ ($M = xz, yz$); higher-order terms with bubbles made of $\chi^c_M(\pm\boldsymbol{Q})$ (= multi-fluctuation process) are relevant. (d) Enhancement of $\Lambda_{ll',ab,ef}$ due to charge VCs.

Here, we find a significant role of the AL term inherent in the multiorbital Hubbard model.

Now, we perform the SC-VC analysis, in the way to satisfy $\hat{\chi}^{c,s}(q)$ in the VC are equal to the total susceptibilities in Eq. (2). Then, $\hat{\chi}^c(q)$ is strongly enhanced by $X^{\mathrm{AL},c}$ in Eq. (5), which is relevant when either $\hat{\chi}^c$ or $\hat{\chi}^s$ is large. On the other hand, we have verified numerically that $\hat{X}^s \sim T\sum \Lambda \cdot V^s V^c \cdot \Lambda$ is less important, although it could be relevant only when both $\hat{\chi}^c$ and $\hat{\chi}^s$ are large. Hereafter, we drop $\hat{X}^s(q)$ to simplify the argument. Figure 3 (a) show $\chi^c_\gamma(\boldsymbol{q})$ given by the SC-VC method for $n = 6.1$, $J/U = 0.088$ and $U = 1.53$, in which the Stoner factors are $\alpha^s_{\max} = \alpha^c_{\mathbf{0}} = 0.97$ and $\alpha^c_{\boldsymbol{Q}} = 0.86$. Compared to the RPA, both $\chi^c_{x^2-y^2}(\boldsymbol{q})$ and $\chi^c_{xz}(\boldsymbol{q})$ are strongly enhanced by the charge AL term, $\hat{X}^{\mathrm{AL},c}$, since the results are essentially unchanged even if MT term is dropped. In the SC-VC method, the enhancements of other charge multipole susceptibilities are small. Especially, both the density and dipole susceptibilities, $\sum_{l,m}\hat{\chi}^c_{ll,mm}(\boldsymbol{q})$ and $\chi^c_\mu(q)$ ($\mu = x, y, z$) respectively, are suppressed.

Here, we discuss the importance of the AL term: At $\boldsymbol{q} \approx \mathbf{0}$ or $\boldsymbol{Q}$, $\chi^c_\gamma(\boldsymbol{q})$ is enlarged by the diagonal vertex correction with respect to γ, $X^{\mathrm{AL},c}_\gamma(\boldsymbol{q}) \equiv \mathrm{Tr}\{\hat{O}_\gamma \hat{X}^{\mathrm{AL},c}(\boldsymbol{q})\hat{O}_\gamma\}/\mathrm{Tr}\{\hat{O}^2_\gamma\}$, since the off-diagonal terms are absent or small [28]. The charge AL term in Eq. (5) is given by the products of two χ^c's (two-orbiton process) and two χ^s's (two-magnon process), shown in Fig. 2 (b). The former process was discussed in Ref. [28], and the latter has a similarity to the spin nematic theory in Ref. [16] based on a frustrated spin model. Now, we consider the orbital selection rule for the two-orbiton process: Because of the relation $\mathrm{Tr}\{\hat{O}_{x^2-y^2}\hat{O}^2_M\} \neq 0$ for $M = xz, yz$ and a rough relation $\Lambda_{ll',ab,cd} \sim \Lambda_{ll',l'b,bl}\delta_{l',a}\delta_{b,c}\delta_{d,l}$ [28], the two-orbiton process for $\gamma = x^2 - y^2$ is mainly given by $\chi^c_M(\boldsymbol{Q})^2$. According to Eq. (5) and Ref. [28], $X^{\mathrm{AL},c}_{x^2-y^2}(\mathbf{0}) \sim \Lambda^2 U^4 T \sum_q \{\chi(q)\}^2$ grows in proportion to $T\chi(\boldsymbol{Q})$ [$\log\{\chi(\boldsymbol{Q})\}^2$] at high [low] temperatures. In the case of Fig. 3 (a), two-magnon process is more important for $\chi^c_{x^2-y^2}(\mathbf{0})$ because of the relation $\alpha^s_{\boldsymbol{Q}} > \alpha^c_{\boldsymbol{Q}}$. We checked that the two-magnon process is mainly caused by $\chi^s_{22,22}(\boldsymbol{Q})^2 - \chi^s_{22,33}(\boldsymbol{Q})^2 > 0$.

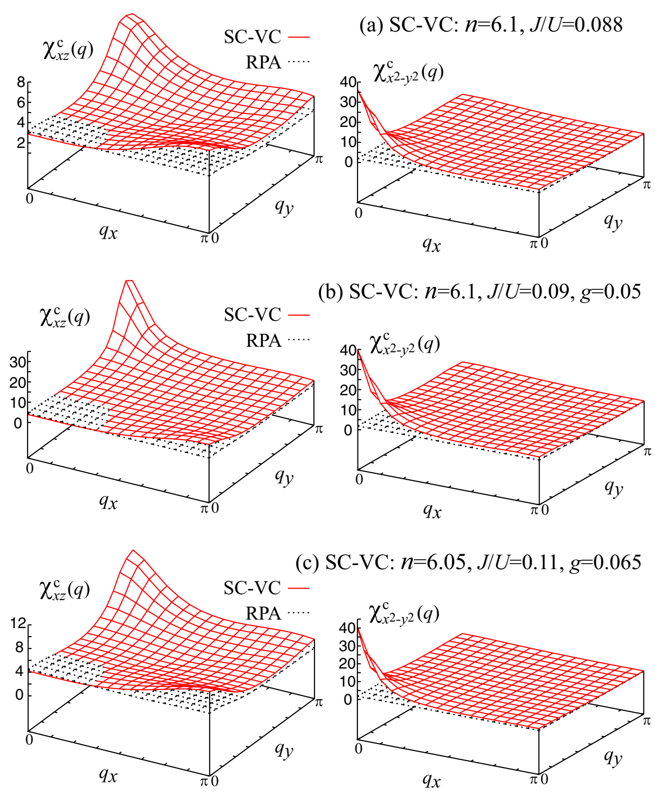

FIG. 3: (color online) $\chi^c_{xz}(\boldsymbol{q})$ and $\chi^c_{x^2-y^2}(\boldsymbol{q})$ given by the SC-VC method. The relation $\alpha^s_{\max} = \alpha^c_{\mathbf{0}} = 0.97$ is satisfied in all cases: (a) $n = 6.1$ and $J/U = 0.88$ ($\alpha^c_{\boldsymbol{Q}} = 0.86$), (b) $n = 6.1$, $J/U = 0.9$ and $g = 0.05$ ($\alpha^c_{\boldsymbol{Q}} = 0.96$), and (c) $n = 6.05$, $J/U = 0.11$ and $g = 0.065$ ($\alpha^c_{\boldsymbol{Q}} = 0.87$).

In the same way, $X^c_M(\boldsymbol{Q}) \sim \Lambda^2 U^4 T \sum_q \chi^c_M(q + Q)\chi^c_{x^2-y^2}(q)$ is enlarged by the two-orbiton process due to $\chi^c_M(\boldsymbol{Q})$ and $\chi^c_{x^2-y^2}(\mathbf{0})$, shown in Fig. 2 (c). (In this case, two-magnon process is less important since $\chi^s(\mathbf{0})$ is small.) The obtained $\chi^c_{xz}(\boldsymbol{q})$ has peaks at $\boldsymbol{q} = \boldsymbol{Q}$ and $\boldsymbol{Q}'$ since the inter-orbital scattering is emphasized by $X^c_{xz}(\boldsymbol{Q}) \propto \chi^c_{x^2-y^2}(\mathbf{0}) \gg 1$. Thus, both $\chi^c_{xz}(\boldsymbol{Q})$ and $\chi^c_{x^2-y^2}(\mathbf{0})$ are strongly enlarged in the SC-VC method, because of the "positive feedback" brought by these two

AL terms: Figure 2 (c) shows an example of the higher-order terms that are automatically generated in the SC-VC method. Such "multi-fluctuation processes" inherent in the self-consistent method magnify the RPA results.

Thus, strong ferro- and AF-orbital fluctuations are caused by AL terms. Both fluctuations work as the pairing interaction for the s_{++}-state, while the ferro-fluctuations are also favorable for the $s_{\pm}$-state. For $J/U < (J/U)_c \equiv 0.088$, the relation $\alpha^s_{\rm max} < \alpha^c_{\mathbf{0}} = 0.97$ is realized and $\alpha^c_{\boldsymbol{Q}}$ increases towards unity. In this case, orbital order occurs prior to the spin order as increasing U with J/U is fixed, since the VC (due to two-orbiton process) can efficiently enlarge orbital susceptibilities because of large $\alpha^c_{\rm max}$(RPA). This situation would be consistent with wider non-magnetic orthorhombic phase in Nd(Fe,Co)As and many 1111 compounds.

Since the present SC-VC method is very time-consuming, we applied some simplifications: We have verified in the self-inconsistent calculation that $\mathrm{Tr}\{\hat{O}_\gamma \hat{X}(q) \hat{O}_{\gamma'}\}$ with $\gamma \neq \gamma'$ is zero or very small, especially at $\boldsymbol{q} = \mathbf{0}$ and $\boldsymbol{Q}$ for the reason of symmetry. Since we are interested in the enhancement of $\chi^c_\gamma(\boldsymbol{q})$ at $\boldsymbol{q} = \mathbf{0}$ and $\boldsymbol{Q}$ and the dominant interferences between $\gamma = xz, yz, x^2-y^2$, we calculated $X_{ll',mm'}(q)$ only for $\{(l,l'),(m,m')\} \in xz, yz, x^2-y^2$. [$(l,l') \in \gamma$ means that $O^{l,l'}_\gamma \neq 0$.] That is, $\{(l,l'),(m,m')\} = \{(1,2),(3,4),(2,5)\}$, $\{(1,3),(2,4),(3,5)\}$, and $\{(1,5),(2,2),(3,3)\}$.

We stress that both $(J/U)_c$ and AF-orbital fluctuations increase by considering following two factors: The first one is the charge VC at each point of the three-point vertex in Fig. 2 (d), as a consequence of the Ward identity between $\hat{\Lambda}$ and $\hat{\chi}^{\rm irr}$. The enhancement factor at each point is estimated as $1 + X^c_\gamma/\chi^0_\gamma = 1.3 \sim 2.5$ for $\gamma = xz$ and x^2-y^2 in the present calculation near the critical point. This effect will increase $(J/U)_c$ sensitively. The second factor is the e-ph interaction: We introduce the quadrupole interaction in Eq. (1) due to Fe-ion oscillations [6, 14, 27]. As shown in Fig. 3 (b), very strong AF-orbital fluctuations are obtained for $J/U = 0.09$ and $g = 0.05$; $\alpha^s_{\rm max} = \alpha^c_{\mathbf{0}} = 0.97$ and $\alpha^c_{\boldsymbol{Q}} = 0.96$. The corresponding dimensionless coupling is just $\lambda = gN(0) \sim 0.035$ [6, 27]. We also study the case $n = 6.05$ and $g = 0.065$, and find that the relation $\alpha^s_{\rm max} = \alpha^c_{\rm max} = 0.97$ is realized at $(J/U)_c = 0.11$, as shown in Fig. 3 (c). For these reasons, strong ferro- and AF-orbital-fluctuations would be realized by the cooperation of the Coulomb and weak e-ph interactions.

Finally, we make some comments: The present multi-fluctuation mechanism is not described by the dynamical-mean-field theory (DMFT), since the irreducible VC is treated as *local*. Also, the local density approximation (LDA), in which the VC is neglected, does not reproduce the nonmagnetic orthorhombic phase. Although Yanagi *et al.* studied $U' > U$ model [7] based on the RPA, that was first studied in Ref. [31], $\chi^c_{3z^2-r^2}(\mathbf{0})$ develops while $\chi^c_{x^2-y^2}(\mathbf{0})$ remains small, inconsistently with the structure transition. Our important future issue is to include the electron self-energy correction into the SC-VC method, which is important to discuss the filling and T-dependences of orbital and spin fluctuations, and to obtain more reliable $(J/U)_c$.

In summary, we developed the SC-VC method, and obtained the Coulomb-interaction-driven nematic and AF-orbital fluctuations due to the multimode (orbitons+magnons) interference effect [28] that is overlooked in the RPA. For $J/U \lesssim (J/U)_c$, the structure transition ($\alpha^c_{\mathbf{0}} \approx 1$) occurs prior to the magnetic transition ($\alpha^s_{\boldsymbol{Q}} \approx 1$), consistently with experiments. When $\alpha^s_{\rm max} \sim \alpha^c_{\rm max}$, both s_{++}- and $s_{\pm}$-states could be realized, depending on model parameters like the impurity concentration [3, 6]. In a sense of the renormalization group scheme, the quadrupole interaction in Eq. (1) is induced by the Coulomb interaction beyond the RPA. We expect that orbital-fluctuation-mediated superconductivity and structure transition are realized in many iron-based superconductors due to the cooperation of the Coulomb and e-ph interactions.

This study has been supported by Grants-in-Aid for Scientific Research from MEXT of Japan, and by JST, TRIP. Part of numerical calculations were performed on the Yukawa Institute Computer Facility.

[1] K. Kuroki *et al.*, Phys. Rev. Lett. **101**, 087004 (2008).
[2] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. **101**, 057003 (2008).
[3] P. J. Hirschfeld, *et al.*, Rep. Prog. Phys. **74**, 124508 (2011).
[4] A. V. Chubukov, arXiv:1110.0052.
[5] F. Wang *et al.*, Phys. Rev. Lett. **102**, 047005 (2009): The used parameters are $U = 4$, $U' = 2$ and $J = 0.7$eV.
[6] H. Kontani and S. Onari, Phys. Rev. Lett. **104**, 157001 (2010).
[7] Y. Yanagi *et al.*, Phys. Rev. B **81**, 054518 (2010).
[8] M. Sato *et al.*, J. Phys. Soc. Jpn. **79** (2009) 014710; S. C. Lee *et al.*, J. Phys. Soc. Jpn. **79** (2010) 023702.
[9] Y. Nakajima *et al.*, Phys. Rev. B **82**, 220504 (2010).
[10] J. Li *et al.*, Phys. Rev. B **84**, 020513(R) (2011); J. Li *et al.*, Phys. Rev. B **85**, 214509 (2012).
[11] K. Kirshenbaum *et al.*, arXiv:1203.5114.
[12] S. Onari and H. Kontani, Phys. Rev. Lett. **103** 177001 (2009).
[13] T. Shimojima *et al.*, Sccience **332**, 564 (2011).
[14] T. Saito *et al.* Phys. Rev. B **82**, 144510 (2010).
[15] S. Onari *et al.*, Phys. Rev. B **81**, 060504(R) (2010); S. Onari and H. Kontani, Phys. Rev. B **84**, 144518 (2011).
[16] R.M. Fernandes *et al.*, Phys. Rev. Lett. **105**, 157003 (2010).
[17] T. Goto *et al.*, J. Phys. Soc. Jpn. **80**, 073702 (2011).
[18] M. Yoshizawa *et al.*, Phys. Soc. Jpn. **81**, 024604 (2012).
[19] J.L. Niedziela *et al.*, Phys. Rev. B **84**, 224305 (2011).
[20] M. Yi *et al.*, PNAS **108** 6878.
[21] Y. K. Kim *et al.*, arXiv:1112.2243.

[22] I. R. Fisher *et al.*, Rep. Prog. Phys. **74** 124506 (2011).
[23] S. Kasahara *et al.*, Nature **486**, 382 (2012).
[24] Y. Inoue *et al.*, Phys. Rev. B **85**, 224506 (2012).
[25] C.-C. Lee *et al.*, Phys. Rev. Lett. **103**, 267001 (2009); W. Lv *et al.*, Phys. Rev. B **82**, 045125 (2010); K. Sugimoto *et al.*, J. Phys. Soc. Jpn. **80** (2011) 033706.
[26] T. Miyake *et al.*, J. Phys. Soc. Jpn. 79, 044705 (2010).
[27] S. Onari and H. Kontani, Phys. Rev. B **85**, 134507 (2012).
[28] H. Kontani *et al.*, Phys. Rev. B **84**, 024528 (2011).
[29] T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer-Verlag, 1985); A. Kawabata: J. Phys. F **4** (1974) 1477.
[30] N. E. Bickers and S. R. White Phys. Rev. B **43**, 8044 (1991); K. Morita *et al.*, J. Phy. Soc. Jpn. **72**, 3164 (2003).
[31] T. Takimoto *et al.*, J. Phys.: Condens. Matter **14**, L369 (2002).